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THERMODYNAMICS OF COAL CONVERSION REACTIONS

PART 3. THE BOUDARD REACTION

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COAL CONVERSION SECTION

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PART 3. The Boudard Reaction

INTRODUCTION

In the Boudard reaction carbon dioxide reacts with carbon to produce carbon monoxide.

$$C + CO_2 \rightarrow 2CO \qquad (1)$$

Because this reaction plays an important role in coal gasification it was felt that a small report summarizing the thermodynamics of this reaction might be useful. The reaction is endothermic (about 41.2 kcal as written above). Thermodynamic data for this report were taken from Ref. (1) because they are believed to be reliable and are set forth in a convenient form for using. For each substance the free energy, ΔF, is set out as a polynomial function of temperature, in degrees Kelvin. Obtaining the free energy change for a reaction is simply a matter of addition and subtraction of the appropriate terms. The equation derived for the free energy-temperature relationship was:

$$F = A + B \ln T + CT^2 + D/T + ET \quad (T \text{ in } {}^{o}K)$$

The values of the parameters A,B,C,D and E for these calculations using this equation are given at the end of Appendix A.

Having derived the free energy change for the reaction at a particular temperature, the equilibrium content, K was calculated from the relationship,

$$\Delta F = -RT \ln K$$

$$\ln K = -\Delta F/RT$$

$$\text{i.e. } K = \text{ExP } (\ln K)$$

The equilibrium constant for this reaction can be expressed in simple form as,

$$K = \frac{P^2CO}{PCO}, \text{ consuming activity of carbon} = 1.$$

The equilibrium, and the gas composition in the system will be affected by the pressure. Considering the system to consist of carbon (graphite) and the two gases CO and CO_2, the total pressure will consist of $PCO + PCO_2$.

$$\text{i.e. } P = PCO + PCO_2$$

$$PCO_2 = P - PCO$$

$$K = \frac{P^2CO}{P-PCO}$$

This can be reduced to

$$P^2CO + K\ PCO - KP = 0$$

This quadratic equation can be solved as,

$$PCO = \frac{-K + \sqrt{K^2 + 4KP}}{2}$$

If XCO is the mol fraction of CO in the gas mixture, then XCO = PCO/P.

A Fortran program was written for the NOVA minicomputer, and executed using pressures of 1, 10, 50 and 100 atmospheres. The results are tabulated in Appendices A, B, C and D respectively.

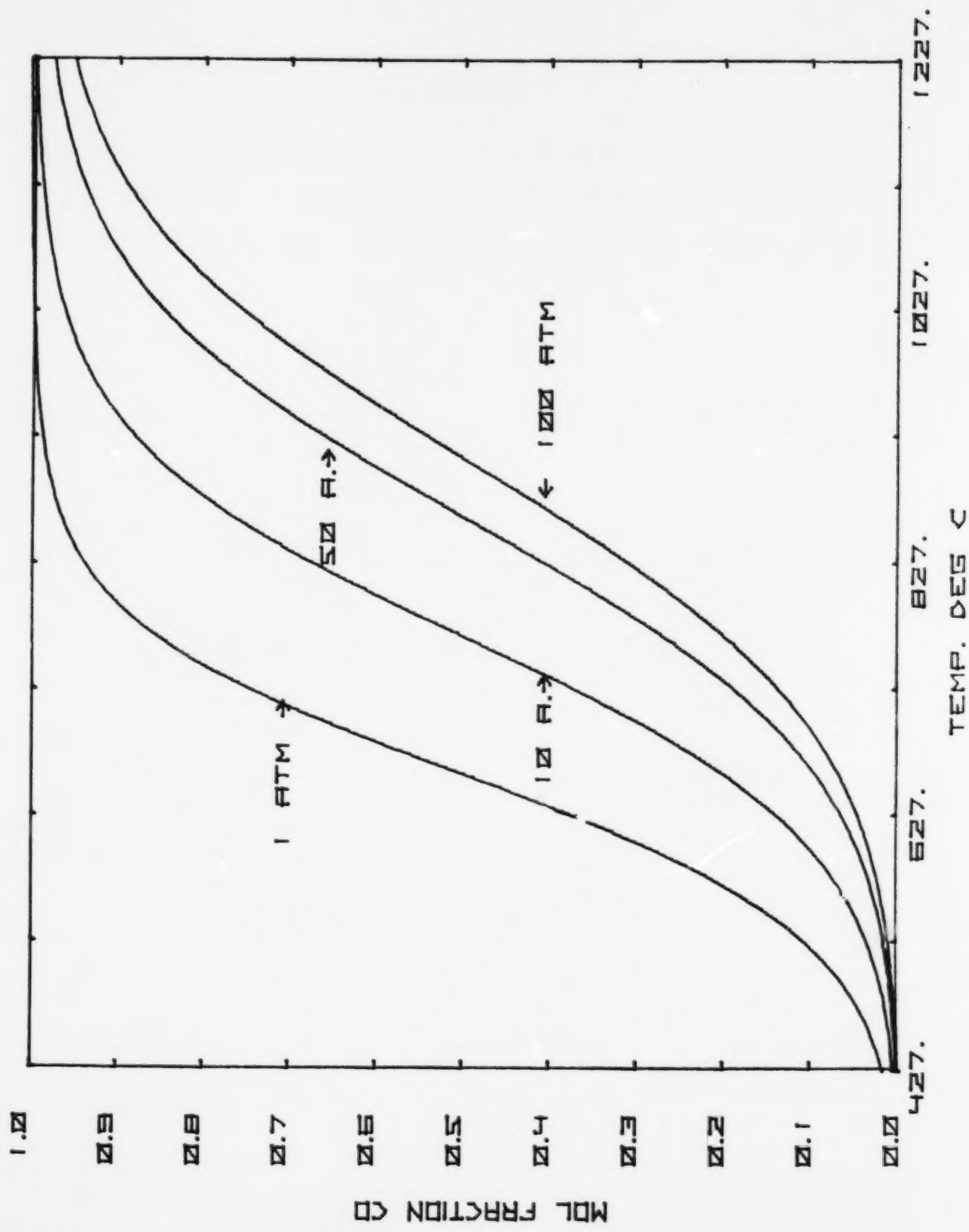

Figure 1. Mol-Fraction of C0 in Boudard Reaction as a Function of Temperature and Pressure.

In addition to having the tabulated data, it often is useful to see a relationship such as this in graphic form. Consequently, the program was written and run on the Hewlett-Packard calculator and plotted. The result is shown in Figure 1.

DISCUSSION

It is evident from Figure 1 that at one atmosphere pressure, the mol-fraction of CO in the mixture increases rapidly from virtually zero at about 427°C (700°K) to reach a value of 1 at a temperature of about 1027°C (1300°K). At higher total pressure, the increase in CO content is not as rapid, and higher temperatures are needed to achieve the same amount of CO in the gas. For instance, CO mol-fraction of 0.8 could be achieved at about 750°C at 1 atm, but would need about 880°C at 10 atm, about 1000°C at 50 atm, and about 1050°C at 100 atm.

It must be remembered that this is a pure thermodynamic analysis of the Boudard reaction alone. What actually happends in a real gasification situation will undoubtedly be affected by kinetic factors and computing reactions.

REFERENCES

1. Wicks, C.E. and Block, F.E. "Thermodynamic properties of 65 elements - Their oxides, halides, carbides and nitrides" U.S.B.M. Bull 605. U.S. Government Printing Office, 1963.

APPENDIX A

Mol-Fraction of CO in Boudard Reaction at One Atmosphere Total Pressure

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
332.	605.	15401.	-12.82	.27191E -5	0.00	1.00
337.	610.	15187.	-12.53	.36055E -5	0.00	1.00
342.	615.	14972.	-12.26	.47587E -5	0.00	1.00
347.	620.	14758.	-11.98	.62525E -5	0.00	1.00
352.	625.	14543.	-11.71	.81793E -5	0.00	1.00
357.	630.	14329.	-11.45	.10654E -4	0.00	1.00
362.	635.	14114.	-11.19	.13819E -4	0.00	1.00
367.	640.	13900.	-10.93	.17852E -4	0.00	1.00
372.	645.	13686.	-10.68	.22970E -4	0.00	1.00
377.	650.	13471.	-10.43	.29439E -4	0.01	0.99
382.	655.	13257.	-10.19	.37587E -4	0.01	0.99
387.	660.	13043.	-9.95	.47811E -4	0.00	0.99
392.	665.	12829.	-9.71	.60595E -4	0.00	0.99
397.	670.	12614.	-9.48	.76525E -4	0.00	0.99
402.	675.	12400.	-9.25	.96305E -4	0.01	0.99
407.	680.	12186.	-9.02	.12079E -3	0.01	0.99
412.	685.	11972.	-8.80	.15098E -3	0.01	0.99
417.	690.	11758.	-8.58	.18812E -3	0.01	0.99
422.	695.	11544.	-8.36	.23364E -3	0.02	0.98
427.	700.	11330.	-8.15	.28927E -3	0.02	0.98
432.	705.	11116.	-7.94	.35706E -3	0.02	0.98
437.	710.	10902.	-7.73	.43940E -3	0.02	0.98
442.	715.	10689.	-7.53	.53916E -3	0.02	0.98
447.	720.	10475.	-7.32	.65968E -3	0.03	0.97
452.	725.	10261.	-7.12	.80486E -3	0.03	0.97
457.	730.	10047.	-6.93	.97930E -3	0.03	0.97
462.	735.	9834.	-6.74	.11883E -2	0.03	0.97
467.	740.	9620.	-6.54	.14382E -2	0.04	0.96
472.	745.	9407.	-6.36	.17360E -2	0.04	0.96
477.	750.	9193.	-6.17	.20903E -2	0.04	0.96
482.	755.	8980.	-5.99	.25106E -2	0.05	0.95
487.	760.	8766.	-5.81	.30080E -2	0.05	0.95
492.	765.	8553.	-5.63	.35954E -2	0.06	0.94
497.	770.	8339.	-5.45	.42874E -2	0.06	0.94
502.	775.	8126.	-5.28	.51009E -2	0.06	0.93
507.	780.	7913.	-5.11	.60551E -2	0.07	0.93
512.	785.	7700.	-4.94	.71718E -2	0.08	0.92
517.	790.	7486.	-4.77	.84761E -2	0.08	0.91
522.	795.	7273.	-4.61	.99963E -2	0.09	0.90
527.	800.	7060.	-4.44	.11765E -1	0.10	0.90
532.	805.	6847.	-4.28	.13817E -1	0.11	0.89
537.	810.	6634.	-4.12	.16195E -1	0.12	0.88
542.	815.	6421.	-3.97	.18945E -1	0.13	0.87
547.	820.	6208.	-3.81	.22119E -1	0.14	0.86
552.	825.	5995.	-3.66	.25776E -1	0.15	0.85
557.	830.	5783.	-3.51	.29981E -1	0.16	0.84
562.	835.	5570.	-3.36	.34807E -1	0.17	0.83
567.	840.	5357.	-3.21	.40338E -1	0.18	0.82
572.	845.	5144.	-3.06	.46666E -1	0.19	0.81
577.	850.	4932.	-2.92	.53891E -1	0.21	0.79

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
582.	855.	4719.	-2.78	.62129E -1	0.22	0.78
587.	860.	4507.	-2.64	.71506E -1	0.23	0.77
592.	865.	4294.	-2.50	.82163E -1	0.25	0.75
597.	870.	4082.	-2.36	.94254E -1	0.26	0.74
602.	875.	3869.	-2.23	.10795E 0	0.28	0.72
607.	880.	3657.	-2.09	.12345E 0	0.30	0.70
612.	885.	3445.	-1.96	.14095E 0	0.31	0.69
617.	890.	3232.	-1.83	.16069E 0	0.33	0.67
622.	895.	3020.	-1.70	.18292E 0	0.35	0.65
627.	900.	2808.	-1.57	.20793E 0	0.36	0.64
632.	905.	2596.	-1.44	.23600E 0	0.38	0.62
637.	910.	2384.	-1.32	.26750E 0	0.40	0.60
642.	915.	2172.	-1.19	.30277E 0	0.42	0.58
647.	920.	1960.	-1.07	.34222E 0	0.44	0.56
652.	925.	1748.	-0.95	.38629E 0	0.46	0.54
657.	930.	1536.	-0.83	.43546E 0	0.48	0.52
662.	935.	1324.	-0.71	.49025E 0	0.50	0.50
667.	940.	1112.	-0.60	.55122E 0	0.52	0.48
672.	945.	900.	-0.48	.61899E 0	0.54	0.46
677.	950.	689.	-0.36	.69422E 0	0.56	0.44
682.	955.	477.	-0.25	.77765E 0	0.57	0.43
687.	960.	265.	-0.14	.87004E 0	0.59	0.41
692.	965.	54.	-0.03	.97227E 0	0.61	0.39
697.	970.	-158.	0.08	.10852E 1	0.63	0.37
702.	975.	-369.	0.19	.12099E 1	0.65	0.35
707.	980.	-580.	0.30	.13474E 1	0.67	0.33
712.	985.	-792.	0.40	.14989E 1	0.69	0.31
717.	990.	-1003.	0.51	.16655E 1	0.70	0.30
722.	995.	-1214.	0.61	.18486E 1	0.72	0.28
727.	1000.	-1426.	0.72	.20497E 1	0.74	0.26
732.	1005.	-1637.	0.82	.22703E 1	0.75	0.25
737.	1010.	-1848.	0.92	.25120E 1	0.77	0.23
742.	1015.	-2059.	1.02	.27767E 1	0.78	0.22
747.	1020.	-2270.	1.12	.30661E 1	0.79	0.21
752.	1025.	-2481.	1.22	.33823E 1	0.81	0.19
757.	1030.	-2692.	1.32	.37275E 1	0.82	0.18
762.	1035.	-2903.	1.41	.41040E 1	0.83	0.17
767.	1040.	-3114.	1.51	.45143E 1	0.84	0.16
772.	1045.	-3325.	1.60	.49609E 1	0.85	0.15
777.	1050.	-3535.	1.70	.54467E 1	0.86	0.14
782.	1055.	-3746.	1.79	.59746E 1	0.87	0.13
787.	1060.	-3957.	1.88	.65478E 1	0.88	0.12
792.	1065.	-4167.	1.97	.71697E 1	0.89	0.11
797.	1070.	-4378.	2.06	.78438E 1	0.90	0.10
802.	1075.	-4588.	2.15	.85739E 1	0.90	0.09
807.	1080.	-4799.	2.24	.93641E 1	0.91	0.08
812.	1085.	-5009.	2.32	.10219E 2	0.92	0.08
817.	1090.	-5220.	2.41	.11142E 2	0.92	0.07
822.	1095.	-5430.	2.50	.12139E 2	0.93	0.07
827.	1100.	-5640.	2.58	.13214E 2	0.93	0.06

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
832.	1105.	-5851.	2.67	.14373E 2	0.94	0.06
837.	1110.	-6061.	2.75	.15622E 2	0.94	0.06
842.	1115.	-6271.	2.83	.16967E 2	0.95	0.05
847.	1120.	-6481.	2.91	.18413E 2	0.95	0.05
852.	1125.	-6691.	2.99	.19967E 2	0.95	0.05
857.	1130.	-6901.	3.07	.21636E 2	0.96	0.04
862.	1135.	-7111.	3.15	.23429E 2	0.96	0.04
867.	1140.	-7321.	3.23	.25351E 2	0.96	0.04
872.	1145.	-7531.	3.31	.27411E 2	0.97	0.03
877.	1150.	-7741.	3.39	.29619E 2	0.97	0.03
882.	1155.	-7950.	3.47	.31982E 2	0.97	0.03
887.	1160.	-8160.	3.54	.34510E 2	0.97	0.03
892.	1165.	-8370.	3.62	.37212E 2	0.97	0.03
897.	1170.	-8579.	3.69	.40100E 2	0.98	0.02
902.	1175.	-8789.	3.77	.43183E 2	0.98	0.02
907.	1180.	-8998.	3.84	.46474E 2	0.98	0.02
912.	1185.	-9208.	3.91	.49983E 2	0.98	0.02
917.	1190.	-9417.	3.98	.53723E 2	0.98	0.02
922.	1195.	-9627.	4.06	.57707E 2	0.98	0.02
927.	1200.	-9836.	4.13	.61948E 2	0.98	0.02
932.	1205.	-10045.	4.20	.66461E 2	0.99	0.01
937.	1210.	-10255.	4.27	.71259E 2	0.99	0.01
942.	1215.	-10464.	4.34	.76359E 2	0.99	0.01
947.	1220.	-10673.	4.40	.81775E 2	0.99	0.01
952.	1225.	-10882.	4.47	.87525E 2	0.99	0.01
957.	1230.	-11091.	4.54	.93626E 2	0.99	0.01
962.	1235.	-11300.	4.61	.10010E 3	0.99	0.01
967.	1240.	-11509.	4.67	.10695E 3	0.99	0.00
972.	1245.	-11718.	4.74	.11422E 3	0.99	0.00
977.	1250.	-11927.	4.80	.12191E 3	0.99	0.00
982.	1255.	-12136.	4.87	.13005E 3	0.99	0.00
987.	1260.	-12344.	4.93	.13865E 3	0.99	0.00
992.	1265.	-12553.	5.00	.14775E 3	0.99	0.00
997.	1270.	-12762.	5.06	.15737E 3	0.99	0.00
1002.	1275.	-12971.	5.12	.16753E 3	0.99	0.01
1007.	1280.	-13179.	5.18	.17825E 3	0.99	0.01
1012.	1285.	-13388.	5.24	.18956E 3	0.99	0.01
1017.	1290.	-13596.	5.31	.20149E 3	1.00	0.00
1022.	1295.	-13805.	5.37	.21406E 3	1.00	0.00
1027.	1300.	-14013.	5.43	.22731E 3	1.00	0.00
1032.	1305.	-14221.	5.49	.24127E 3	1.00	0.00
1037.	1310.	-14430.	5.55	.25596E 3	1.00	0.00
1042.	1315.	-14638.	5.60	.27142E 3	1.00	0.00
1047.	1320.	-14846.	5.66	.28768E 3	1.00	0.00
1052.	1325.	-15054.	5.72	.30477E 3	1.00	0.00
1057.	1330.	-15262.	5.78	.32274E 3	1.00	0.00
1062.	1335.	-15471.	5.83	.34161E 3	1.00	0.00
1067.	1340.	-15679.	5.89	.36142E 3	1.00	0.00
1072.	1345.	-15887.	5.95	.38222E 3	1.00	0.00
1077.	1350.	-16094.	6.00	.40404E 3	1.00	0.00

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
1082.	1355.	-16302.	6.06	.42692E 3	1.00	0.00
1087.	1360.	-16510.	6.11	.45091E 3	1.00	0.00
1092.	1365.	-16718.	6.17	.47605E 3	1.00	0.00
1097.	1370.	-16926.	6.22	.50238E 3	1.00	0.00
1102.	1375.	-17133.	6.27	.52995E 3	1.00	0.00
1107.	1380.	-17341.	6.33	.55881E 3	1.00	0.00
1112.	1385.	-17549.	6.38	.58900E 3	1.00	0.00
1117.	1390.	-17756.	6.43	.62058E 3	1.00	0.00
1122.	1395.	-17964.	6.48	.65360E 3	1.00	0.00
1127.	1400.	-18171.	6.53	.68811E 3	1.00	0.00
1132.	1405.	-18379.	6.59	.72416E 3	1.00	0.00
1137.	1410.	-18586.	6.64	.76181E 3	1.00	0.00
1142.	1415.	-18793.	6.69	.80112E 3	1.00	0.00
1147.	1420.	-19001.	6.74	.84215E 3	1.00	0.00
1152.	1425.	-19208.	6.79	.88496E 3	1.00	0.00
1157.	1430.	-19415.	6.83	.92960E 3	1.00	0.00
1162.	1435.	-19622.	6.88	.97614E 3	1.00	0.00
1167.	1440.	-19829.	6.93	.10247E 4	1.00	0.00
1172.	1445.	-20036.	6.98	.10752E 4	1.00	0.00
1177.	1450.	-20243.	7.03	.11278E 4	1.00	0.00
1182.	1455.	-20450.	7.08	.11827E 4	1.00	0.00
1187.	1460.	-20657.	7.12	.12397E 4	1.00	0.00
1192.	1465.	-20864.	7.17	.12991E 4	1.00	0.00
1197.	1470.	-21071.	7.22	.13608E 4	1.00	0.00
1202.	1475.	-21278.	7.26	.14251E 4	1.00	0.00
1207.	1480.	-21485.	7.31	.14918E 4	1.00	0.00
1212.	1485.	-21691.	7.35	.15612E 4	1.00	0.00
1217.	1490.	-21898.	7.40	.16333E 4	1.00	0.00
1222.	1495.	-22105.	7.44	.17082E 4	1.00	0.00
1227.	1500.	-22311.	7.49	.17859E 4	1.00	0.00
1232.	1505.	-22518.	7.53	.18666E 4	1.00	0.00
1237.	1510.	-22724.	7.58	.19504E 4	1.00	0.00
1242.	1515.	-22931.	7.62	.20373E 4	1.00	0.00
1247.	1520.	-23137.	7.66	.21274E 4	1.00	0.00
1252.	1525.	-23343.	7.71	.22209E 4	1.00	0.00
1257.	1530.	-23550.	7.75	.23177E 4	1.00	0.00
1262.	1535.	-23756.	7.79	.24181E 4	1.00	0.00
1267.	1540.	-23962.	7.83	.25221E 4	1.00	0.00
1272.	1545.	-24168.	7.87	.26298E 4	1.00	0.00
1277.	1550.	-24374.	7.92	.27414E 4	1.00	0.00
1282.	1555.	-24580.	7.96	.28568E 4	1.00	0.00
1287.	1560.	-24786.	8.00	.29763E 4	1.00	0.00
1292.	1565.	-24992.	8.04	.30999E 4	1.00	0.00
1297.	1570.	-25198.	8.08	.32278E 4	1.00	0.00
1302.	1575.	-25404.	8.12	.33601E 4	1.00	0.00
1307.	1580.	-25610.	8.16	.34968E 4	1.00	0.00
1312.	1585.	-25816.	8.20	.36381E 4	1.00	0.00
1317.	1590.	-26021.	8.24	.37842E 4	1.00	0.00
1322.	1595.	-26227.	8.28	.39351E 4	1.00	0.00
1327.	1600.	-26433.	8.32	.40909E 4	1.00	0.00

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
1332.	1605.	-26638.	8.36	.42518E 4	1.00	0.00

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 A=        42890.0000
 B=            1.0700
 C=          0.00061
 D=    -197000.0000
 E =         -52.1200

EQUATION: F = A + B*T*LN(T) + C*T *T + D/T + E*T
STOP
R
```

APPENDIX B

Mol-Fraction of CO in Boudard Reaction at 10 Atmospheres Total Pressure

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
427.	700.	11330.	-8.15	.28927E -3	0.01	0.99
432.	705.	11116.	-7.94	.35706E -3	0.01	0.99
437.	710.	10902.	-7.73	.43940E -3	0.00	0.99
442.	715.	10689.	-7.53	.53916E -3	0.00	0.99
447.	720.	10475.	-7.32	.65968E -3	0.00	0.99
452.	725.	10261.	-7.12	.80486E -3	0.00	0.99
457.	730.	10047.	-6.93	.97930E -3	0.01	0.99
462.	735.	9834.	-6.74	.11883E -2	0.01	0.99
467.	740.	9620.	-6.54	.14382E -2	0.01	0.99
472.	745.	9407.	-6.36	.17360E -2	0.01	0.99
477.	750.	9193.	-6.17	.20903E -2	0.01	0.99
482.	755.	8980.	-5.99	.25106E -2	0.02	0.98
487.	760.	8766.	-5.81	.30080E -2	0.02	0.98
492.	765.	8553.	-5.63	.35954E -2	0.02	0.98
497.	770.	8339.	-5.45	.42874E -2	0.02	0.98
502.	775.	8126.	-5.28	.51009E -2	0.02	0.98
507.	780.	7913.	-5.11	.60551E -2	0.02	0.98
512.	785.	7700.	-4.94	.71718E -2	0.03	0.97
517.	790.	7486.	-4.77	.84761E -2	0.03	0.97
522.	795.	7273.	-4.61	.99963E -2	0.03	0.97
527.	800.	7060.	-4.44	.11765E -1	0.03	0.97
532.	805.	6847.	-4.28	.13817E -1	0.04	0.96
537.	810.	6634.	-4.12	.16195E -1	0.04	0.96
542.	815.	6421.	-3.97	.18945E -1	0.04	0.96
547.	820.	6208.	-3.81	.22119E -1	0.05	0.95
552.	825.	5995.	-3.66	.25776E -1	0.05	0.95
557.	830.	5783.	-3.51	.29981E -1	0.05	0.95
562.	835.	5570.	-3.36	.34807E -1	0.06	0.94
567.	840.	5357.	-3.21	.40338E -1	0.06	0.94
572.	845.	5144.	-3.06	.46666E -1	0.06	0.93
577.	850.	4932.	-2.92	.53891E -1	0.07	0.93
582.	855.	4719.	-2.78	.62129E -1	0.07	0.92
587.	860.	4507.	-2.64	.71506E -1	0.08	0.92
592.	865.	4294.	-2.50	.82163E -1	0.08	0.91
597.	870.	4082.	-2.36	.94254E -1	0.09	0.91
602.	875.	3869.	-2.23	.10795E 0	0.09	0.90
607.	880.	3657.	-2.09	.12345E 0	0.11	0.89
612.	885.	3445.	-1.96	.14095E 0	0.11	0.89
617.	890.	3232.	-1.83	.16069E 0	0.12	0.88
622.	895.	3020.	-1.70	.18292E 0	0.13	0.87
627.	900.	2808.	-1.57	.20793E 0	0.13	0.87
632.	905.	2596.	-1.44	.23600E 0	0.14	0.86
637.	910.	2384.	-1.32	.26750E 0	0.15	0.85
642.	915.	2172.	-1.19	.30277E 0	0.16	0.84
647.	920.	1960.	-1.07	.34222E 0	0.17	0.83
652.	925.	1748.	-0.95	.38629E 0	0.18	0.82
657.	930.	1536.	-0.83	.43546E 0	0.19	0.81
662.	935.	1324.	-0.71	.49025E 0	0.20	0.80
667.	940.	1112.	-0.60	.55122E 0	0.21	0.79
672.	945.	900.	-0.48	.61899E 0	0.22	0.78

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K		XCO	XCO2
677.	950.	689.	-0.36	.69422E	0	0.23	0.77
682.	955.	477.	-0.25	.77765E	0	0.24	0.76
687.	960.	265.	-0.14	.87004E	0	0.25	0.75
692.	965.	54.	-0.03	.97227E	0	0.27	0.73
697.	970.	-158.	0.08	.10852E	1	0.28	0.72
702.	975.	-369.	0.19	.12099E	1	0.29	0.71
707.	980.	-580.	0.30	.13474E	1	0.31	0.69
712.	985.	-792.	0.40	.14989E	1	0.32	0.68
717.	990.	-1003.	0.51	.16655E	1	0.33	0.67
722.	995.	-1214.	0.61	.18486E	1	0.35	0.65
727.	1000.	-1426.	0.72	.20497E	1	0.36	0.64
732.	1005.	-1637.	0.82	.22703E	1	0.38	0.62
737.	1010.	-1848.	0.92	.25120E	1	0.39	0.61
742.	1015.	-2059.	1.02	.27767E	1	0.41	0.59
747.	1020.	-2270.	1.12	.30661E	1	0.42	0.58
752.	1025.	-2481.	1.22	.33823E	1	0.44	0.56
757.	1030.	-2692.	1.32	.37275E	1	0.45	0.55
762.	1035.	-2903.	1.41	.41040E	1	0.47	0.53
767.	1040.	-3114.	1.51	.45143E	1	0.48	0.52
772.	1045.	-3325.	1.60	.49609E	1	0.50	0.50
777.	1050.	-3535.	1.70	.54467E	1	0.51	0.49
782.	1055.	-3746.	1.79	.59746E	1	0.53	0.47
787.	1060.	-3957.	1.88	.65478E	1	0.55	0.45
792.	1065.	-4167.	1.97	.71697E	1	0.56	0.44
797.	1070.	-4378.	2.06	.78438E	1	0.58	0.42
802.	1075.	-4588.	2.15	.85739E	1	0.59	0.41
807.	1080.	-4799.	2.24	.93641E	1	0.61	0.39
812.	1085.	-5009.	2.32	.10219E	2	0.62	0.38
817.	1090.	-5220.	2.41	.11142E	2	0.64	0.36
822.	1095.	-5430.	2.50	.12139E	2	0.65	0.35
827.	1100.	-5640.	2.58	.13214E	2	0.67	0.33
832.	1105.	-5851.	2.67	.14373E	2	0.68	0.32
837.	1110.	-6061.	2.75	.15622E	2	0.69	0.31
842.	1115.	-6271.	2.83	.16967E	2	0.71	0.29
847.	1120.	-6481.	2.91	.18413E	2	0.72	0.28
852.	1125.	-6691.	2.99	.19967E	2	0.73	0.27
857.	1130.	-6901.	3.07	.21636E	2	0.74	0.26
862.	1135.	-7111.	3.15	.23429E	2	0.76	0.24
867.	1140.	-7321.	3.23	.25351E	2	0.77	0.23
872.	1145.	-7531.	3.31	.27411E	2	0.78	0.22
877.	1150.	-7741.	3.39	.29619E	2	0.79	0.21
882.	1155.	-7950.	3.47	.31982E	2	0.80	0.20
887.	1160.	-8160.	3.54	.34510E	2	0.81	0.19
892.	1165.	-8370.	3.62	.37212E	2	0.82	0.18
897.	1170.	-8579.	3.69	.40100E	2	0.83	0.17
902.	1175.	-8789.	3.77	.43183E	2	0.84	0.16
907.	1180.	-8998.	3.84	.46474E	2	0.85	0.15
912.	1185.	-9208.	3.91	.49983E	2	0.85	0.15
917.	1190.	-9417.	3.98	.53723E	2	0.86	0.14
922.	1195.	-9627.	4.06	.57707E	2	0.87	0.13

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
927.	1200.	-9836.	4.13	.61948E 2	0.88	0.12
932.	1205.	-10045.	4.20	.66461E 2	0.88	0.12
937.	1210.	-10255.	4.27	.71259E 2	0.89	0.11
942.	1215.	-10464.	4.34	.76359E 2	0.90	0.10
947.	1220.	-10673.	4.40	.81775E 2	0.90	0.09
952.	1225.	-10882.	4.47	.87525E 2	0.91	0.09
957.	1230.	-11091.	4.54	.93626E 2	0.91	0.08
962.	1235.	-11300.	4.61	.10010E 3	0.92	0.08
967.	1240.	-11509.	4.67	.10695E 3	0.92	0.07
972.	1245.	-11718.	4.74	.11422E 3	0.93	0.07
977.	1250.	-11927.	4.80	.12191E 3	0.93	0.07
982.	1255.	-12136.	4.87	.13005E 3	0.93	0.06
987.	1260.	-12344.	4.93	.13865E 3	0.94	0.06
992.	1265.	-12553.	5.00	.14775E 3	0.94	0.06
997.	1270.	-12762.	5.06	.15737E 3	0.94	0.06
1002.	1275.	-12971.	5.12	.16753E 3	0.95	0.05
1007.	1280.	-13179.	5.18	.17825E 3	0.95	0.05
1012.	1285.	-13388.	5.24	.18956E 3	0.95	0.05
1017.	1290.	-13596.	5.31	.20149E 3	0.95	0.05
1022.	1295.	-13805.	5.37	.21406E 3	0.96	0.04
1027.	1300.	-14013.	5.43	.22731E 3	0.96	0.04
1032.	1305.	-14221.	5.49	.24127E 3	0.96	0.04
1037.	1310.	-14430.	5.55	.25596E 3	0.96	0.04
1042.	1315.	-14638.	5.60	.27142E 3	0.97	0.03
1047.	1320.	-14846.	5.66	.28768E 3	0.97	0.03
1052.	1325.	-15054.	5.72	.30477E 3	0.97	0.03
1057.	1330.	-15262.	5.78	.32274E 3	0.97	0.03
1062.	1335.	-15471.	5.83	.34161E 3	0.97	0.03
1067.	1340.	-15679.	5.89	.36142E 3	0.97	0.03
1072.	1345.	-15887.	5.95	.38222E 3	0.98	0.02
1077.	1350.	-16094.	6.00	.40404E 3	0.98	0.02
1082.	1355.	-16302.	6.06	.42692E 3	0.98	0.02
1087.	1360.	-16510.	6.11	.45091E 3	0.98	0.02
1092.	1365.	-16718.	6.17	.47605E 3	0.98	0.02
1097.	1370.	-16926.	6.22	.50238E 3	0.98	0.02
1102.	1375.	-17133.	6.27	.52995E 3	0.98	0.02
1107.	1380.	-17341.	6.33	.55881E 3	0.98	0.02
1112.	1385.	-17549.	6.38	.58900E 3	0.98	0.02
1117.	1390.	-17756.	6.43	.62058E 3	0.98	0.02
1122.	1395.	-17964.	6.48	.65360E 3	0.99	0.01
1127.	1400.	-18171.	6.53	.68811E 3	0.99	0.01
1132.	1405.	-18379.	6.59	.72416E 3	0.99	0.01
1137.	1410.	-18586.	6.64	.76181E 3	0.99	0.01
1142.	1415.	-18793.	6.69	.80112E 3	0.99	0.01
1147.	1420.	-19001.	6.74	.84215E 3	0.99	0.01
1152.	1425.	-19208.	6.79	.88496E 3	0.99	0.01
1157.	1430.	-19415.	6.83	.92960E 3	0.99	0.01
1162.	1435.	-19622.	6.88	.97614E 3	0.99	0.01
1167.	1440.	-19829.	6.93	.10247E 4	0.99	0.01
1172.	1445.	-20036.	6.98	.10752E 4	0.99	0.00

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
1177.	1450.	-20243.	7.03	.11278E 4	0.99	0.00
1182.	1455.	-20450.	7.08	.11827E 4	0.99	0.00
1187.	1460.	-20657.	7.12	.12397E 4	0.99	0.00
1192.	1465.	-20864.	7.17	.12991E 4	0.99	0.00
1197.	1470.	-21071.	7.22	.13608E 4	0.99	0.00
1202.	1475.	-21278.	7.26	.14251E 4	0.99	0.00
1207.	1480.	-21485.	7.31	.14918E 4	0.99	0.00
1212.	1485.	-21691.	7.35	.15612E 4	0.99	0.00
1217.	1490.	-21898.	7.40	.16333E 4	0.99	0.01
1222.	1495.	-22105.	7.44	.17082E 4	0.99	0.01
1227.	1500.	-22311.	7.49	.17859E 4	0.99	0.01
1232.	1505.	-22518.	7.53	.18666E 4	0.99	0.01

```
A=        42890.0000
B=            1.0700
C=          0.00061
D=    -197000.0000
E =         -52.1200

EQUATION: F = A + B*T*LN(T) + C*T *T + D/T + E*T
STOP
R
```

APPENDIX C

Mol-Fraction of CO in Boudard Reaction at 50 Atmospheres Total Pressure

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
432.	705.	11116.	-7.94	.35706E -3	0.00	1.00
437.	710.	10902.	-7.73	.43940E -3	0.00	1.00
442.	715.	10689.	-7.53	.53916E -3	0.00	1.00
447.	720.	10475.	-7.32	.65968E -3	0.00	1.00
452.	725.	10261.	-7.12	.80486E -3	0.00	1.00
457.	730.	10047.	-6.93	.97930E -3	0.00	1.00
462.	735.	9834.	-6.74	.11883E -2	0.00	1.00
467.	740.	9620.	-6.54	.14382E -2	0.01	0.99
472.	745.	9407.	-6.36	.17360E -2	0.01	0.99
477.	750.	9193.	-6.17	.20903E -2	0.00	0.99
482.	755.	8980.	-5.99	.25106E -2	0.00	0.99
487.	760.	8766.	-5.81	.30080E -2	0.00	0.99
492.	765.	8553.	-5.63	.35954E -2	0.00	0.99
497.	770.	8339.	-5.45	.42874E -2	0.00	0.99
502.	775.	8126.	-5.28	.51009E -2	0.01	0.99
507.	780.	7913.	-5.11	.60551E -2	0.01	0.99
512.	785.	7700.	-4.94	.71718E -2	0.01	0.99
517.	790.	7486.	-4.77	.84761E -2	0.01	0.99
522.	795.	7273.	-4.61	.99963E -2	0.01	0.99
527.	800.	7060.	-4.44	.11765E -1	0.02	0.98
532.	805.	6847.	-4.28	.13817E -1	0.02	0.98
537.	810.	6634.	-4.12	.16195E -1	0.02	0.98
542.	815.	6421.	-3.97	.18945E -1	0.02	0.98
547.	820.	6208.	-3.81	.22119E -1	0.02	0.98
552.	825.	5995.	-3.66	.25776E -1	0.02	0.98
557.	830.	5783.	-3.51	.29981E -1	0.02	0.98
562.	835.	5570.	-3.36	.34807E -1	0.03	0.97
567.	840.	5357.	-3.21	.40338E -1	0.03	0.97
572.	845.	5144.	-3.06	.46666E -1	0.03	0.97
577.	850.	4932.	-2.92	.53891E -1	0.03	0.97
582.	855.	4719.	-2.78	.62129E -1	0.03	0.97
587.	860.	4507.	-2.64	.71506E -1	0.04	0.96
592.	865.	4294.	-2.50	.82163E -1	0.04	0.96
597.	870.	4082.	-2.36	.94254E -1	0.04	0.96
602.	875.	3869.	-2.23	.10795E 0	0.05	0.95
607.	880.	3657.	-2.09	.12345E 0	0.05	0.95
612.	885.	3445.	-1.96	.14095E 0	0.05	0.95
617.	890.	3232.	-1.83	.16069E 0	0.06	0.94
622.	895.	3020.	-1.70	.18292E 0	0.06	0.94
627.	900.	2808.	-1.57	.20793E 0	0.06	0.94
632.	905.	2596.	-1.44	.23600E 0	0.06	0.93
637.	910.	2384.	-1.32	.26750E 0	0.07	0.93
642.	915.	2172.	-1.19	.30277E 0	0.07	0.93
647.	920.	1960.	-1.07	.34222E 0	0.07	0.92
652.	925.	1748.	-0.95	.38629E 0	0.08	0.92
657.	930.	1536.	-0.83	.43546E 0	0.08	0.91
662.	935.	1324.	-0.71	.49025E 0	0.09	0.91
667.	940.	1112.	-0.60	.55122E 0	0.10	0.90
672.	945.	900.	-0.48	.61899E 0	0.11	0.89
677.	950.	689.	-0.36	.69422E 0	0.11	0.89

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
682.	955.	477.	-0.25	.77765E 0	0.12	0.88
687.	960.	265.	-0.14	.87004E 0	0.12	0.88
692.	965.	54.	-0.03	.97227E 0	0.13	0.87
697.	970.	-158.	0.08	.10852E 1	0.14	0.86
702.	975.	-369.	0.19	.12099E 1	0.14	0.86
707.	980.	-580.	0.30	.13474E 1	0.15	0.85
712.	985.	-792.	0.40	.14989E 1	0.16	0.84
717.	990.	-1003.	0.51	.16655E 1	0.17	0.83
722.	995.	-1214.	0.61	.18486E 1	0.17	0.83
727.	1000.	-1426.	0.72	.20497E 1	0.18	0.82
732.	1005.	-1637.	0.82	.22703E 1	0.19	0.81
737.	1010.	-1848.	0.92	.25120E 1	0.20	0.80
742.	1015.	-2059.	1.02	.27767E 1	0.21	0.79
747.	1020.	-2270.	1.12	.30661E 1	0.22	0.78
752.	1025.	-2481.	1.22	.33823E 1	0.23	0.77
757.	1030.	-2692.	1.32	.37275E 1	0.24	0.76
762.	1035.	-2903.	1.41	.41040E 1	0.25	0.75
767.	1040.	-3114.	1.51	.45143E 1	0.26	0.74
772.	1045.	-3325.	1.60	.49609E 1	0.27	0.73
777.	1050.	-3535.	1.70	.54467E 1	0.28	0.72
782.	1055.	-3746.	1.79	.59746E 1	0.29	0.71
787.	1060.	-3957.	1.88	.65478E 1	0.30	0.70
792.	1065.	-4167.	1.97	.71697E 1	0.31	0.69
797.	1070.	-4378.	2.06	.78438E 1	0.33	0.67
802.	1075.	-4588.	2.15	.85739E 1	0.34	0.66
807.	1080.	-4799.	2.24	.93641E 1	0.35	0.65
812.	1085.	-5009.	2.32	.10219E 2	0.36	0.64
817.	1090.	-5220.	2.41	.11142E 2	0.37	0.63
822.	1095.	-5430.	2.50	.12139E 2	0.39	0.61
827.	1100.	-5640.	2.58	.13214E 2	0.40	0.60
832.	1105.	-5851.	2.67	.14373E 2	0.41	0.59
837.	1110.	-6061.	2.75	.15622E 2	0.42	0.58
842.	1115.	-6271.	2.83	.16967E 2	0.44	0.56
847.	1120.	-6481.	2.91	.18413E 2	0.45	0.55
852.	1125.	-6691.	2.99	.19967E 2	0.46	0.54
857.	1130.	-6901.	3.07	.21636E 2	0.48	0.52
862.	1135.	-7111.	3.15	.23429E 2	0.49	0.51
867.	1140.	-7321.	3.23	.25351E 2	0.50	0.50
872.	1145.	-7531.	3.31	.27411E 2	0.52	0.48
877.	1150.	-7741.	3.39	.29619E 2	0.53	0.47
882.	1155.	-7950.	3.47	.31982E 2	0.54	0.46
887.	1160.	-8160.	3.54	.34510E 2	0.55	0.45
892.	1165.	-8370.	3.62	.37212E 2	0.57	0.43
897.	1170.	-8579.	3.69	.40100E 2	0.58	0.42
902.	1175.	-8789.	3.77	.43183E 2	0.59	0.41
907.	1180.	-8998.	3.84	.46474E 2	0.61	0.39
912.	1185.	-9208.	3.91	.49983E 2	0.62	0.38
917.	1190.	-9417.	3.98	.53723E 2	0.63	0.37
922.	1195.	-9627.	4.06	.57707E 2	0.64	0.36
927.	1200.	-9836.	4.13	.61948E 2	0.65	0.35

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
932.	1205.	-10045.	4.20	.66461E 2	0.67	0.33
937.	1210.	-10255.	4.27	.71259E 2	0.68	0.32
942.	1215.	-10464.	4.34	.76359E 2	0.69	0.31
947.	1220.	-10673.	4.40	.81775E 2	0.70	0.30
952.	1225.	-10882.	4.47	.87525E 2	0.71	0.29
957.	1230.	-11091.	4.54	.93626E 2	0.72	0.28
962.	1235.	-11300.	4.61	.10010E 3	0.73	0.27
967.	1240.	-11509.	4.67	.10695E 3	0.74	0.26
972.	1245.	-11718.	4.74	.11422E 3	0.75	0.25
977.	1250.	-11927.	4.80	.12191E 3	0.76	0.24
982.	1255.	-12136.	4.87	.13005E 3	0.77	0.23
987.	1260.	-12344.	4.93	.13865E 3	0.78	0.22
992.	1265.	-12553.	5.00	.14775E 3	0.79	0.21
997.	1270.	-12762.	5.06	.15737E 3	0.80	0.20
1002.	1275.	-12971.	5.12	.16753E 3	0.81	0.19
1007.	1280.	-13179.	5.18	.17825E 3	0.81	0.19
1012.	1285.	-13388.	5.24	.18956E 3	0.82	0.18
1017.	1290.	-13596.	5.31	.20149E 3	0.83	0.17
1022.	1295.	-13805.	5.37	.21406E 3	0.84	0.16
1027.	1300.	-14013.	5.43	.22731E 3	0.84	0.16
1032.	1305.	-14221.	5.49	.24127E 3	0.85	0.15
1037.	1310.	-14430.	5.55	.25596E 3	0.86	0.14
1042.	1315.	-14638.	5.60	.27142E 3	0.86	0.14
1047.	1320.	-14846.	5.66	.28768E 3	0.87	0.13
1052.	1325.	-15054.	5.72	.30477E 3	0.87	0.13
1057.	1330.	-15262.	5.78	.32274E 3	0.88	0.12
1062.	1335.	-15471.	5.83	.34161E 3	0.89	0.11
1067.	1340.	-15679.	5.89	.36142E 3	0.89	0.11
1072.	1345.	-15887.	5.95	.38222E 3	0.90	0.10
1077.	1350.	-16094.	6.00	.40404E 3	0.90	0.10
1082.	1355.	-16302.	6.06	.42692E 3	0.90	0.09
1087.	1360.	-16510.	6.11	.45091E 3	0.91	0.09
1092.	1365.	-16718.	6.17	.47605E 3	0.91	0.08
1097.	1370.	-16926.	6.22	.50238E 3	0.92	0.08
1102.	1375.	-17133.	6.27	.52995E 3	0.92	0.08
1107.	1380.	-17341.	6.33	.55881E 3	0.92	0.07
1112.	1385.	-17549.	6.38	.58900E 3	0.93	0.07
1117.	1390.	-17756.	6.43	.62058E 3	0.93	0.07
1122.	1395.	-17964.	6.48	.65360E 3	0.93	0.06
1127.	1400.	-18171.	6.53	.68811E 3	0.94	0.06
1132.	1405.	-18379.	6.59	.72416E 3	0.94	0.06
1137.	1410.	-18586.	6.64	.76181E 3	0.94	0.06
1142.	1415.	-18793.	6.69	.80112E 3	0.94	0.06
1147.	1420.	-19001.	6.74	.84215E 3	0.95	0.05
1152.	1425.	-19208.	6.79	.88496E 3	0.95	0.05
1157.	1430.	-19415.	6.83	.92960E 3	0.95	0.05
1162.	1435.	-19622.	6.88	.97614E 3	0.95	0.05
1167.	1440.	-19829.	6.93	.10247E 4	0.96	0.04
1172.	1445.	-20036.	6.98	.10752E 4	0.96	0.04
1177.	1450.	-20243.	7.03	.11278E 4	0.96	0.04

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
1182.	1455.	-20450.	7.08	.11827E 4	0.96	0.04
1187.	1460.	-20657.	7.12	.12397E 4	0.96	0.04
1192.	1465.	-20864.	7.17	.12991E 4	0.96	0.04
1197.	1470.	-21071.	7.22	.13608E 4	0.97	0.03
1202.	1475.	-21278.	7.26	.14251E 4	0.97	0.03
1207.	1480.	-21485.	7.31	.14918E 4	0.97	0.03
1212.	1485.	-21691.	7.35	.15612E 4	0.97	0.03
1217.	1490.	-21898.	7.40	.16333E 4	0.97	0.03
1222.	1495.	-22105.	7.44	.17082E 4	0.97	0.03
1227.	1500.	-22311.	7.49	.17859E 4	0.97	0.03

```
A=        42890.0000
B=            1.0700
C=          0.00061
D=    -197000.0000
E =         -52.1200

EQUATION: F = A + B*T*LN(T) + C*T *T + D/T + E*T
STOP
R
```

APPENDIX D

Mol-Fraction of CO in Boudard Reaction at 100 Atmospheres Total Pressure

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
532.	805.	6847.	-4.28	.13817E -1	0.01	0.99
537.	810.	6634.	-4.12	.16195E -1	0.01	0.99
542.	815.	6421.	-3.97	.18945E -1	0.01	0.99
547.	820.	6208.	-3.81	.22119E -1	0.01	0.99
552.	825.	5995.	-3.65	.25776E -1	0.02	0.98
557.	830.	5783.	-3.51	.29981E -1	0.02	0.98
562.	835.	5570.	-3.36	.34807E -1	0.02	0.98
567.	840.	5357.	-3.21	.40338E -1	0.02	0.98
572.	845.	5144.	-3.06	.46656E -1	0.02	0.98
577.	850.	4932.	-2.92	.53891E -1	0.02	0.98
582.	855.	4719.	-2.78	.62129E -1	0.02	0.98
587.	860.	4507.	-2.64	.71506E -1	0.03	0.97
592.	865.	4294.	-2.50	.82163E -1	0.03	0.97
597.	870.	4082.	-2.36	.94254E -1	0.03	0.97
602.	875.	3869.	-2.23	.10795E 0	0.03	0.97
607.	880.	3657.	-2.09	.12345E 0	0.03	0.97
612.	885.	3445.	-1.96	.14095E 0	0.04	0.96
617.	890.	3232.	-1.83	.16069E 0	0.04	0.96
622.	895.	3020.	-1.70	.18292E 0	0.04	0.96
627.	900.	2808.	-1.57	.20793E 0	0.04	0.96
632.	905.	2596.	-1.44	.23600E 0	0.05	0.95
637.	910.	2384.	-1.32	.26750E 0	0.05	0.95
642.	915.	2172.	-1.19	.30277E 0	0.05	0.95
647.	920.	1960.	-1.07	.34222E 0	0.06	0.94
652.	925.	1748.	-0.95	.38629E 0	0.06	0.94
657.	930.	1536.	-0.83	.43546E 0	0.06	0.94
662.	935.	1324.	-0.71	.49025E 0	0.06	0.93
667.	940.	1112.	-0.60	.55122E 0	0.07	0.93
672.	945.	900.	-0.48	.61899E 0	0.07	0.92
677.	950.	689.	-0.36	.69422E 0	0.08	0.92
682.	955.	477.	-0.25	.77765E 0	0.08	0.92
687.	960.	265.	-0.14	.87004E 0	0.08	0.91
692.	965.	54.	-0.03	.97227E 0	0.09	0.91
697.	970.	-158.	0.08	.10852E 1	0.09	0.90
702.	975.	-369.	0.19	.12099E 1	0.10	0.90
707.	980.	-580.	0.30	.13474E 1	0.11	0.89
712.	985.	-792.	0.40	.14989E 1	0.12	0.88
717.	990.	-1003.	0.51	.16655E 1	0.12	0.88
722.	995.	-1214.	0.61	.18486E 1	0.13	0.87
727.	1000.	-1426.	0.72	.20497E 1	0.13	0.87
732.	1005.	-1637.	0.82	.22703E 1	0.14	0.86
737.	1010.	-1848.	0.92	.25120E 1	0.15	0.85
742.	1015.	-2059.	1.02	.27767E 1	0.15	0.85
747.	1020.	-2270.	1.12	.30661E 1	0.16	0.84
752.	1025.	-2481.	1.22	.33823E 1	0.17	0.83
757.	1030.	-2692.	1.32	.37275E 1	0.18	0.82
762.	1035.	-2903.	1.41	.41040E 1	0.18	0.82
767.	1040.	-3114.	1.51	.45143E 1	0.19	0.81
772.	1045.	-3325.	1.60	.49609E 1	0.20	0.80
777.	1050.	-3535.	1.70	.54467E 1	0.21	0.79

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
782.	1055.	-3746.	1.79	.59746E 1	0.22	0.78
787.	1060.	-3957.	1.88	.65478E 1	0.23	0.77
792.	1065.	-4167.	1.97	.71697E 1	0.23	0.77
797.	1070.	-4378.	2.06	.78438E 1	0.24	0.76
802.	1075.	-4588.	2.15	.85739E 1	0.25	0.75
807.	1080.	-4799.	2.24	.93641E 1	0.26	0.74
812.	1085.	-5009.	2.32	.10219E 2	0.27	0.73
817.	1090.	-5220.	2.41	.11142E 2	0.28	0.72
822.	1095.	-5430.	2.50	.12139E 2	0.29	0.71
827.	1100.	-5640.	2.58	.13214E 2	0.30	0.70
832.	1105.	-5851.	2.67	.14373E 2	0.31	0.69
837.	1110.	-6061.	2.75	.15622E 2	0.32	0.68
842.	1115.	-6271.	2.83	.16967E 2	0.34	0.66
847.	1120.	-6481.	2.91	.18413E 2	0.35	0.65
852.	1125.	-6691.	2.99	.19967E 2	0.36	0.64
857.	1130.	-6901.	3.07	.21636E 2	0.37	0.63
862.	1135.	-7111.	3.15	.23429E 2	0.38	0.62
867.	1140.	-7321.	3.23	.25351E 2	0.39	0.61
872.	1145.	-7531.	3.31	.27411E 2	0.40	0.60
877.	1150.	-7741.	3.39	.29619E 2	0.42	0.58
882.	1155.	-7950.	3.47	.31982E 2	0.43	0.57
887.	1160.	-8160.	3.54	.34510E 2	0.44	0.56
892.	1165.	-8370.	3.62	.37212E 2	0.45	0.55
897.	1170.	-8579.	3.69	.40100E 2	0.46	0.54
902.	1175.	-8789.	3.77	.43183E 2	0.48	0.52
907.	1180.	-8998.	3.84	.46474E 2	0.49	0.51
912.	1185.	-9208.	3.91	.49983E 2	0.50	0.50
917.	1190.	-9417.	3.98	.53723E 2	0.51	0.49
922.	1195.	-9627.	4.06	.57707E 2	0.52	0.48
927.	1200.	-9836.	4.13	.61948E 2	0.54	0.46
932.	1205.	-10045.	4.20	.66461E 2	0.55	0.45
937.	1210.	-10255.	4.27	.71259E 2	0.56	0.44
942.	1215.	-10464.	4.34	.76359E 2	0.57	0.43
947.	1220.	-10673.	4.40	.81775E 2	0.58	0.42
952.	1225.	-10882.	4.47	.87525E 2	0.60	0.40
957.	1230.	-11091.	4.54	.93626E 2	0.61	0.39
962.	1235.	-11300.	4.61	.10010E 3	0.62	0.38
967.	1240.	-11509.	4.67	.10695E 3	0.63	0.37
972.	1245.	-11718.	4.74	.11422E 3	0.64	0.36
977.	1250.	-11927.	4.80	.12191E 3	0.65	0.35
982.	1255.	-12136.	4.87	.13005E 3	0.66	0.34
987.	1260.	-12344.	4.93	.13865E 3	0.67	0.33
992.	1265.	-12553.	5.00	.14775E 3	0.68	0.32
997.	1270.	-12762.	5.06	.15737E 3	0.69	0.31
1002.	1275.	-12971.	5.12	.16753E 3	0.70	0.30
1007.	1280.	-13179.	5.18	.17825E 3	0.71	0.29
1012.	1285.	-13388.	5.24	.18956E 3	0.72	0.28
1017.	1290.	-13596.	5.31	.20149E 3	0.73	0.27
1022.	1295.	-13805.	5.37	.21406E 3	0.74	0.26
1027.	1300.	-14013.	5.43	.22731E 3	0.75	0.25

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
1032.	1305.	-14221.	5.49	.24127E 3	0.76	0.24
1037.	1310.	-14430.	5.55	.25596E 3	0.77	0.23
1042.	1315.	-14638.	5.60	.27142E 3	0.78	0.22
1047.	1320.	-14846.	5.66	.28768E 3	0.79	0.21
1052.	1325.	-15054.	5.72	.30477E 3	0.79	0.21
1057.	1330.	-15262.	5.78	.32274E 3	0.80	0.20
1062.	1335.	-15471.	5.83	.34161E 3	0.81	0.19
1067.	1340.	-15679.	5.89	.36142E 3	0.82	0.18
1072.	1345.	-15887.	5.95	.38222E 3	0.82	0.18
1077.	1350.	-16094.	6.00	.40404E 3	0.83	0.17
1082.	1355.	-16302.	6.06	.42692E 3	0.84	0.16
1087.	1360.	-16510.	6.11	.45091E 3	0.84	0.16
1092.	1365.	-16718.	6.17	.47605E 3	0.85	0.15
1097.	1370.	-16926.	6.22	.50238E 3	0.85	0.15
1102.	1375.	-17133.	6.27	.52995E 3	0.86	0.14
1107.	1380.	-17341.	6.33	.55881E 3	0.87	0.13
1112.	1385.	-17549.	6.38	.58900E 3	0.87	0.13
1117.	1390.	-17756.	6.43	.62058E 3	0.88	0.12
1122.	1395.	-17964.	6.48	.65360E 3	0.88	0.12
1127.	1400.	-18171.	6.53	.68811E 3	0.89	0.11
1132.	1405.	-18379.	6.59	.72416E 3	0.89	0.11
1137.	1410.	-18586.	6.64	.76181E 3	0.89	0.11
1142.	1415.	-18793.	6.69	.80112E 3	0.90	0.10
1147.	1420.	-19001.	6.74	.84215E 3	0.90	0.09
1152.	1425.	-19208.	6.79	.88496E 3	0.91	0.09
1157.	1430.	-19415.	6.83	.92960E 3	0.91	0.08
1162.	1435.	-19622.	6.88	.97614E 3	0.91	0.08
1167.	1440.	-19829.	6.93	.10247E 4	0.92	0.08
1172.	1445.	-20036.	6.98	.10752E 4	0.92	0.07
1177.	1450.	-20243.	7.03	.11278E 4	0.92	0.07
1182.	1455.	-20450.	7.08	.11827E 4	0.93	0.07
1187.	1460.	-20657.	7.12	.12397E 4	0.93	0.07
1192.	1465.	-20864.	7.17	.12991E 4	0.93	0.06
1197.	1470.	-21071.	7.22	.13608E 4	0.94	0.06
1202.	1475.	-21278.	7.26	.14251E 4	0.94	0.06
1207.	1480.	-21485.	7.31	.14918E 4	0.94	0.06
1212.	1485.	-21691.	7.35	.15612E 4	0.94	0.06
1217.	1490.	-21898.	7.40	.16333E 4	0.95	0.05
1222.	1495.	-22105.	7.44	.17082E 4	0.95	0.05
1227.	1500.	-22311.	7.49	.17859E 4	0.95	0.05
1232.	1505.	-22518.	7.53	.18666E 4	0.95	0.05
1237.	1510.	-22724.	7.58	.19504E 4	0.95	0.05
1242.	1515.	-22931.	7.62	.20373E 4	0.96	0.04
1247.	1520.	-23137.	7.66	.21274E 4	0.96	0.04
1252.	1525.	-23343.	7.71	.22209E 4	0.96	0.04
1257.	1530.	-23550.	7.75	.23177E 4	0.96	0.04
1262.	1535.	-23756.	7.79	.24181E 4	0.96	0.04
1267.	1540.	-23962.	7.83	.25221E 4	0.96	0.04
1272.	1545.	-24168.	7.87	.26298E 4	0.96	0.04
1277.	1550.	-24374.	7.92	.27414E 4	0.97	0.03

TEMP. DEG.C	TEMP. DEG.K	FREE ENERGY KCAL/KG-MOL	LNK	K	XCO	XCO2
1282.	1555.	-24580.	7.96	.28568E 4	0.97	0.03
1287.	1560.	-24786.	8.00	.29763E 4	0.97	0.03
1292.	1565.	-24992.	8.04	.30999E 4	0.97	0.03
1297.	1570.	-25198.	8.08	.32278E 4	0.97	0.03
1302.	1575.	-25404.	8.12	.33601E 4	0.97	0.03
1307.	1580.	-25610.	8.16	.34968E 4	0.97	0.03
1312.	1585.	-25816.	8.20	.36381E 4	0.97	0.03
1317.	1590.	-26021.	8.24	.37842E 4	0.97	0.03
1322.	1595.	-26227.	8.28	.39351E 4	0.98	0.02
1327.	1600.	-26433.	8.32	.40909E 4	0.98	0.02
1332.	1605.	-26638.	8.36	.42518E 4	0.98	0.02

```
A=        42890.0000
B=            1.0700
C=          0.00061
D=     -197000.0000
E =         -52.1200

EQUATION: F = A + B*T*LN(T) + C*T *T + D/T + E*T
STOP
R
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